

Optical trap of neutral atoms (12 points)

Optical traps are versatile tools to create ultracold atom systems that nowadays play very important role in quantum physics and are believed to have highly nontrivial applications in technology as well as in quantum measurements. By shining a laser beam onto an assembly of neutral atoms, we are able to capture and cool these atoms. When atoms are cooled to near absolute zero temperature, they reveal the whole fascinating quantum behavior, in particular their Bose-Einstein condensation (BEC).

In this problem you will study basic concepts of an optical trap of neutral atoms and one of the signatures to recognize the BEC in experiments on sodium atoms.

An neutral sodium atom can be well described as a core with positive charge *e* surrounded by a homogenous electron cloud with negative charge *-e.* The mass of the core is much larger than the mass of the electron cloud. In the absence of an external electric field, the core and the cloud centers coincide. The electric field of a laser beam interacts with the positive core as well as the electron cloud of the atom, so an electric dipole is induced. In turn, this induced dipole will interact with the electric field of the laser beam and thereby gives rise to a dipole potential energy of the atom. The atom is said to feel an optical potential. The later depends on the intensity profile $I(\vec{r})$ as well as the frequency of the laser beam in use. By choosing an appropriate laser intensity and frequency, one may form a trap-like potential well to confine the neutral atoms.

We start off by considering the polarization of a neutral atom that is placed in a uniform external electric field $\vec{E}_0=E_0\hat{\vec{u}}$, where \hat{u} is a unit vector and E_0 is the field magnitude. Then, a *dipole moment* $\vec{p}_0=e\ell\hat{u}=0$ $\alpha E_0\hat u$ is induced. Here, ℓ is distance between the negative and positive charge centers, and α is called *polarizability.*

Figure 1. Electron cloud distribution. [1] Spherical distribution of electron cloud about the atomic core; [2] Shifted electron cloud (separation of **+** and **-** within the atom) in an electric field.

1 (1.5 points)

Initially the external field is turned off. Then the field magnitude is increased from zero to E_0 very slowly so that the electric field can be considered effectively time-independent in this question. The instantaneous value of the external field is denoted by $\vec{E} = E \hat{u}$,

1.1 Find the instantaneous power absorbed by the atom from the external field in terms of \vec{E} and $\dot{\vec{p}}$, where $\dot{\vec{p}}$ is the rate change of the induced dipole moment. 0.75pt

1.2 Find the total work done by the external field on the atom when the electric field is increased from zero to $E=E_{0}.$ Hence deduce an expression for the induced dipole potential energy $U_{induced}$ in terms of $\vec{E_o}$ and $\vec{p_o}.$ 0.75pt

Note that when the external electric field is turned off, the electron cloud oscillates with a natural frequency ω_0 due to its inertia and the Coulomb restoring force.

2 (1.0 point)

In the following we will study the case where the neutral atoms are placed in an external laser field that varies in time and space as $\vec{E}(\vec{r},t) = \hat{u}.E_0(\vec{r})$ cos $\,\omega t$. The induced dipole moments \vec{p} will oscillate with the driving laser field frequency ω . It is well known that an oscillating dipole itself emits electromagnetic radiation. By doing so, electron receives some recoil momentum that causes an electromagnetic friction resulting in a phase shift between the applied electric field and the induced dipole moment. Therefore, the induced dipole moment takes the form $\vec{p}(\vec{r},t)$ = $\hat{u}E_0(\vec{r})\alpha(\omega)$ cos $[\omega t+\varphi(\omega)].$ Here, both the polarizability α and the phase shift φ depend on the driving frequency ω . Due to the oscillating nature, all physical quantities of our interest reveal themselves only via the corresponding time-averaged values over a period $2\pi/\omega$ of the laser field. The time-averaged value of a periodically varying quantity is defined as

 $\langle f(t) \rangle = \frac{\omega}{2\pi}$ $2\pi/\omega$ ∫ 0 $f\left(t\right)dt.$ Hereafter, the notation $\langle...\rangle$ means time-average of the enclosed quantity.

Laser intensity $I(\vec r)$ is related to amplitude of the laser electric field E_0 as $I(\vec r)$ $=$ $\frac{\varepsilon_0cE_0^2(\vec r)}{2}$, where ϵ_0 is the permittivity of free space and c is the speed of light.

2.1 Find the induced dipole potential energy $U_{dir}(\vec{r}) = \langle U_{induced}(\vec{r},t) \rangle$ in term of $\alpha,\ \varphi,\ \varepsilon_0,\,c,$ and $I(\vec r).$ 1.0pt

3 (1.0 point)

Besides capturing neutral atoms in the trap via the induced dipole potential energy, the oscillating electric field may cause a scattering force on atoms that arises from absorption and emission of light. The light scattering processes lead either to heating or to losses of atoms from the trap and may be characterized by the scattering rate, that is related to the number of photons scattered by an atom in unit time

and is defined by $\Gamma_{sc}(\vec r) = \frac{\langle P_{abs}(\vec r)\rangle}{\hbar\omega}$. Here, $\langle P_{abs}(\vec r)\rangle$ is the time-averaged power absorbed from the laser field, and $\hbar\omega$ is the photon energy $(\hbar = h/2\pi)$.

4 (2.0 points)

Both quantities U_{dip} and $\Gamma_{sc}(\vec r)$ depend on the polarizability α . In order to calculate the polarizability α , we will adopt the one dimensional oscillator model under the presence of an electric field $\vec{E}(t)$ = $\hat{u}E_0$ cos ωt . Let Ox the axis parallel to the unit vector \hat{u} . In this model motion of the electron is determined by three forces:

i) The restoring force $-m_e\omega_0^2x\cdot\hat u$ that describes the free oscillation with the natural frequency ω_0 corresponding to the atomic optical transition frequency. We use *x* to denote the displacement of the negative charge center from the positive one, which is assumed to be at rest.

ii) The driving force of the laser field $-eE_0cos\omega t.\hat{u}$

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iii) The damping force $-m_e \gamma_\omega \dot{x}.\hat{u}$ that originates from the radiation of the accelerating charge, and is characterized by the frequency-dependent damping rate γ_{ω} .

Therefore, the equation of motion of the electron is given as $\ddot x+\gamma_\omega\dot x+\omega_0^2x=\frac{-eE_0\cos\omega t}{m_e}.$ The solution to this equation is $x = x_0\cos(\omega t + \varphi).$ Here x_0 and φ are to be determined.

4.1 Find the polarizability α in term of $\gamma_\omega,$ $e,$ $m_e,$ ω_0 , and $\omega.$ 2.0pt

5 (1.0 point)

In fact the energy damping rate γ_{ω} is independent of the electron orbits. Therefore we will adopt another simple model where the electron cloud center performs a circular motion in the absence of the laser field but with the frequency ω and speed v . Being accelerated, the electron radiates an electromagnectic wave with power given by the Larmor formula $P_L=\frac{1}{6\pi\varepsilon_0}\frac{e^2a^2}{c^3}$ with a denoting acceleration. The damping force is supposed to be related to the damping rate γ_{ω} as $F_d = -m_e \gamma_{\omega} v$. We also assume that the total energy of the electron is large compared with the energy loss per cycle.

6 (0.5 point)

When the driving frequency ω is close to the natural frequency $\omega_0,$ then the polarizability gets larger, leading to a larger value of the dipole potential as well as an increased scattering rate. Therefore, by considering the ratio $U_{dip}(\vec{r})/\hbar\Gamma_{sc}(\vec{r})$, one can find an appropriate laser frequency to reduce the scattering rate while maintaining a reasonably deep trapping potential.

6.1 Introducing the damping rate at $\omega = \omega_0$, as $\gamma \equiv \gamma_{\omega_0}$, find the ratio $U_{dip}(\vec{r})/\hbar\Gamma_{sc}(\vec{r})$ in terms of $\omega, \omega_{0},$ and $\gamma.$ 0.5pt

7 (1.5 points)

From the above result we can see that it is possible to simultaneously achieve a deep trapping potential and low heating rates by choosing the laser frequency ω not to be too close to the atomic optical transition ω_0 , as well as high laser intensity. Because the scattering rate $\Gamma_{sc} \left(\vec{r} \right)$ is positive, and from the above obtained ratio $U_{dip}(\vec r)/\hbar\Gamma_{sc}(\vec r)$, if $\omega<\omega_0$ then the dipole potential is negative and the atoms are captured in a focused region of laser beam with maximum intensity. Once atoms are captured in the trap, by reducing the trapping well depth to remove high energy atoms, one may cool the confined atom gas to ultracold temperatures, enabling formation of BEC. A breakthrough progress in BEC physics had been achieved with sodium atoms 23 Na in the late nineties (D. M. Stamper-Kurn et al., Phys.Rev.Lett. 80, 2027 (1998)).

The physics of BEC can be understood as follows. In nature, there are two kinds of particles: bosons with integer spin and fermions with half integer spin. Two identical fermions cannot exist in the same quantum state. In contrast, multiple bosons are not forbidden to occupy one quantum state: at ultralow temperatures a large fraction of bosons can condensate into the state with lowest possible energy and form a condensate cloud (condensate bosons), while the rest bosons are in the excited state with higher energy (noncondensate or thermal bosons). Let us analyse a practical example of a dilute gas of sodium atoms, which are bosons, confined in the optical trap created by a Gaussian laser beam (Fig 2a). The laser beam has the wavelength λ corresponding to the frequency ω (with $\omega<\omega_0$). The beam propagates along the z-axis with the intensity profile $I(\rho,z) = \frac{2P}{\pi D(z)^2} \exp\left(-\frac{2\rho^2}{D(z)^2}\right)$, where $\rho=\sqrt{x^2+y^2}$ and the waist

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size is $D\,(z)\,=\,D_0\sqrt{1+z^2/z_R^2}$ with $z_R\,=\,\pi D_0^2/\lambda$ denoting the Rayleigh length. The total laser power P and the beam waist parameter D_0 determine the parameters of the optical trapping potential, one of which is the potential depth U_{depth} . The later is defined by the absolute value of the local minimum of the potential energy, taking as a reference the potential energy energy to be zero at infinity (Fig 2b).

Figure 2. (a) Gaussian beam. The envelope represents the beam waist $D(z)$ at the plane $z = const.$ (Adopted from wikipedia); (b) Illustration of optical trap along x-axis created by a Gaussian beam with $\omega < \omega_0.$ The dashed line corresponds to a harmonic approximation near the trap bottom.

- **7.1** Find the expression for the dipole potential depth U_{depth} in terms of $c, \omega, \omega_0, \gamma, P,$ and $D_0.$ 0.5pt
- **7.2** Given laser power $P = 4$ mW, laser wavelength $\lambda = 985$ nm, $D_0 = 6 \,\mu$ m, and natural wave length for sodium $\lambda_0 = 589 \text{ nm}$, evaluate the potential depth U_{depth} . Express your answer as an equivalent temperature $T_{\rm 0}$, at which thermal energy of the non-trapped atom is equal to the trap depth. 1.0pt

8 (0.5 point)

When the cloud temperature T is much smaller than equivalent temperature $T_{\rm 0}$, the optical potential can be well approximated by a cylindrically symmetric harmonic potential $U_{dip}(\rho,z)=-U_{depth}+\frac{1}{2}m\Omega_\rho^2\rho^2+$ $\frac12 m\Omega_z^2 z^2$, where m is the mass of a sodium atom and $\Omega_\rho,$ Ω_z are oscillation frequencies in the corresponding directions.

8.1 Find the expression for $\Omega_\rho,$ Ω_z in terms of $T_0,$ $m,$ $D_0,$ z_R and $k_B.$ Here k_B is the Boltzmann constant. 0.5pt

Recall that at ultralow temperatures, the sodium atom cloud consists of condensate atoms and thermal atoms. Condensate bosons behave according to the uncertainty principle that can be used for estimating the spatial size or the momentum distribution of the cloud. On the other hand, thermal bosons are described by classical physics, in particular, they obey the Maxwell-Boltzmann distribution law.

We estimate the size of the condensate cloud, that is, the mean distance of the condensate sodium

atoms from the trap center. Moving inside this cloud, each condensate atom has potential energy as well as kinetic energy. The potential energy is a monotonically increasing function of the cloud size, and the particle tries to reduce it to reach the lowest energy level. On the other hand, as the cloud size decreases, the uncertainty principle requires an increase in the particle momentum, that results in an increase of kinetic energy. The particle therefore finds an optimal cloud size to balance the two opposite tendencies of the two different energy contributions.

9 (1.0 point)

For simplicity, let us consider the simplest case of one dimensional trap potential $U(z)=const+\frac{1}{2}m\Omega_z^2z^2.$

In what follows we will figure out how to differentiate the condensate cloud from the thermal one by switching off the confining trap. It is neccesary to capture the image of the cloud density profile.

The thermal gas will show an isotropic Maxwell velocity distribution even if the trap is anisotropic. In contrast, the velocity distribution of a BEC is anisotropic. More precisely, the BEC expands faster along the axis of strong confinement than along the axis of weak confinement. The expansion predominantly occurs in the radial direction, and the initially cigar-shaped condensate becomes pancake-shaped. Therefore the density profile after a long time of flight will be anisotropic and inverted with respect to the shape of the cloud in the trap.

Figure 3. Cloud shape. [1] Before switching off the trap; [2] A very long time after switching off the trap.

10 (2.0 points)

Now we extend the previous results to the three-dimensional potential which is the case of the optical trap in a Gaussian laser beam.

- **10.1** Find the aspect ratio $\frac{z_0}{\rho_0}$ in terms of Ω_ρ , Ω_z , where z_0 and ρ_0 are the initial sizes of the condensate cloud. 0.5pt
- **10.2** When the trap is turned off, the condensate will be expanding in different directions with different initial velocities v_ρ and v_z . Determine the ratio $\frac{v_\rho}{v_z}$ in terms of $\Omega_\rho, \, \Omega_z.$ 0.5pt
- **10.3** Assuming that the velocities of the cloud expansion remain unchanged during the expansion, find aspect ratio of the condensate cloud after a long period of time $\frac {z_L}{\rho_L}$ when the cloud size is much greater than its initial size, that is $z_L \gg z_0$ and $\rho_L \gg \rho_0$. 0.5pt
- **10.4** Same as question 10.3., find the aspect ratio of the thermal cloud after a long period of time $\frac{z_{T,L}}{\rho_{T,L}}$ when the cloud size is much greater than its initial size, that is $z_{T,L}\gg z_0$ and $\rho_{T,L}\gg \rho_0.$ 0.5pt

Space elevator (8.0 points)

Useful mathematics formula:

$e^x = 1 + \frac{x}{1!} + \frac{x^2}{2!} + \frac{x^3}{3!} + \dots$

Presently, the use of rockets is the only viable method of transporting material from Earth to Moon, Mars, and beyond. However, this method of space travel is not so efficient. A space elevator, if it could be built, would provide a completely new technology for space travel (Fig. 1). This is a long structure that is anchored at the equator and reaches a higher altitude than geostationary orbit (GEO). Geostationary orbit is a circular orbit positioned approximately 42300 km from the Earth's center and having a period of the same duration and direction as the rotation of the Earth. An object in this orbit will appear stationary relative to the rotating Earth. The modern ideas of the space elevator were first proposed by Artsutanov (Artsutanov, Y. et al., Science, 158, 946, 1967). However, only modest attention was paid to the subject until Pearson published an inspiring paper "The Orbital Tower: a Spacecraft Launcher Using the Earth's Rotational Energy" (Pearson J., *Acta Astronautica.* Vol. 2, p. 785, 1975). In Pearson's paper, many useful features of the space elevator were pointed out and it was made clear that for the space elevator to ever become a reality, the use of a material that is much stronger but much lighter than steel would be necessary. Due to the lack of such a material, there was little continuation of this research for many years, until the 1990s when carbon nanotubes, a new material composed of hexagonal arrays of carbon atoms, were discovered. In 2003, the Port project (http://www.port.com/) was launched to build and operate a space elevator with current technology.

Figure 1. Space Elevator (adapted from wikipedia).(1) Earth; (2) North pole; (3) Anchored at equator; (4) Climber; (5) Counterweight; (6) Rotates with Earth; (7) Cable; (8) Geostationary orbit altitude.

In this part we will study two designs of a space elevator, mechanical properties of carbon nanotubes, and explore some applications of space elevator. You are given the mass of Earth $M = 5.98 \times 10^{24}$ kg, radius of the Earth $R=6370\;{\rm km}$, geostationary orbit radius $R_G=42300\;{\rm km}$, solar mass $M_S=2\times10^{30}\;{\rm kg}$, orbital radius of the Earth around the Sun $R_E~=~1.5\times 10^8 {\rm km}$ = 1AU (AU – the astronomical unit), the orbital speed of the Earth 30.9 km/s, and the speed of rotation of the Earth around its axis $\omega = 7.27 \times 10^{-5}$ rad/s.

1. The cylindrical space elevator with a uniform cross section (1.5 points)

Let us first consider a space elevator, which is a cylindrical wire with a uniform cross section *A* and is homogeneous with density ρ . It is a cylinder positioned vertically at the equator. Its height is greater

than the height of the geostationary satellite orbit, so that the stress (force per unit area) on the bottom of the cylinder is zero. The cylinder is in tension along its entire length, with the stress adjusting itself so that each element of the cylinder is in equilibrium under the action of the gravitational, centrifugal, and tension forces.

- **1.2** Find the distance from the Earth's center to the point where the stress in the cylinder is maximum. 0.5pt
- **1.3** Find the expression for maximum stress of the cylinder in terms of ρ , R_G , R and the gravitational acceleration q . If the cylinder is made of steel whose density is 7900 $\rm kg/m^3$, tensile strength is 5.0 GPa, evaluate the ratio between the maximum stress and the tensile strength of steel. Tensile strength is the maximum stress a material can withstand. 0.5pt

2. Carbon nanotubes (2.5 points)

Calculation in the previous part shows that in order to build the space elevator, it is neccessary to have light materials with very high tensile strength. Carbon nanotubes are materials that meet such requirements because of strong chemical bondings between very light atoms. Two natural polymorphs of carbon are diamond and graphite. In diamond every carbon atom is surrounded by four nearest neighbor (NN) atoms to form a tetrahedron. Graphite has a layer structure. In each layer, carbon atoms are arranged in a hexagonal plane lattice with three NNs. Although diamond is known as the hardest materials, covalent bondings between carbon atoms in hexagonal layers of graphite is stronger than those between carbon atoms in diamond tetrahedra. Graphite is much softer than diamond because of the van der Waals bonding between carbon atoms of different layers, which is much weaker than covalent bonding.

Figure 2. Graphite structure

Figure 3. Graphene (a) and carbon nanotube (b).

A monatomic layer in graphite is called graphene and has monoatomic thickness. Isolated graphene sheet is not stable and has a tendency to roll up to form carbon spheres or carbon nanotubes. The hexagonal crystal lattice of graphene is depicted in Fig. 4. The distance between two NN carbon atoms is $a = 0.142$ nm and the distance between two closest parallel bondings is $b = 0.246$ nm. Because the covalent bondings between carbon atoms in graphene are very strong, mechanical properties of carbon nanotubes are very special. They have an extremely large Young's modulus and tensile strength, as well as a very light density. Young's modulus is defined as the ratio of the stress along an axis to the strain (ratio of deformation over initial length) along that axis in the range of stress in which Hooke's law holds.

Figure 4. Graphene.

Figure 5. An illustration of a carbon nanotube with 9 carbon-carbon parallel bondings. Note: In this problem, there are 27 carbon-carbon parallel bondings. (1) parallel bond; (2) slanted bond; (3) tube axis.

Now we examine some mechanical properties of a carbon nanotube having 27 carbon-carbon bondings parallel to the tube axis (for an illustration, see Figure 5). The bonding between two carbon atoms can be described by the Morse potential $V(x)=V_0(e^{-4\frac{x}{a}}-2e^{-2\frac{x}{a}}).$ Here $a=0.142\,nm$ is the equilibrium distance between two NN carbon atoms, $V_0 = 4.93 \text{eV}$ is the bonding energy, and x is the displacement of the atom from the equilibrium position. Hereafter, we approximate the Morse potential by a quadratic potential $V(x) = P + Qx^2$. All non-nearest-neighbor interactions are neglected. In this approximation, one can propose that carbon atoms are bonded through "springs" with the spring constant k . Changes in angles between bonds are neglected.

In order to estimate the tensile strength, we assume that when the "spring" connecting carbon atoms has the maximum extension x_{max} the harmonic potential energy equals to the bonding energy.

3. The tapered space elevator with a uniform stress (2.5 points)

In the previous section, the density and the tensile strength of carbon nanotubes have been evaluated theoretically. These evaluated values indeed depend on the specific structure of carbon nanotubes. Nevertheless, the idea of space elevator construction is truly feasible. Now we will study a new space elevator

design of the so-called tapered tower whose cross section varies with height in such a way that both the stress σ and mass density ρ are uniform over the entire tower length. The tower has axial symmetry and is positioned vertically at the equator; its height is greater than the height of the geostationary satellite orbit. Denote the cross sectional area of the tapered tower on the Earth surface by A_s and at geostationary height A_G .

- **3.1** Find the cross section $A(h)$ as a function of distance h up the tower from the ground. 0.5pt
- **3.2** The tower is designed symmetrically so that the cross sections at the two ends are equal, find the distance from the center of the Earth to the upper end of the tower. 0.5pt
- **3.3** The taper ratio is defined as A_G/A_S . Find the taper ratio of the tower made of carbon nanotubes with tensile strength 130 GPa and density $1300 \; \mathrm{kg/m^3}.$ 0.5pt
- **3.4** We can considerably shorten the length of the elevator by terminating it at the upper end by a counterweight of the appropriate mass. Let h_C be the height of the tower relative to the geostationary height, and find the relation of mass m_C of the counterweight and h_C . 1.0pt

4. Applications: launching payload into orbit and spacecraft to the other planets (1.5 points)

The main application of space elevator is the use of the tower's rotational energy to launch payload into orbit or send spacecraft to the other planets. It is very easy to get payload into space: we simply have to make it ride up the elevator to an altitude *r* and release it from rest. For simplicity in the calculations, let us assume that the motion of the tower occurs in the plane of Earth's orbit.

4.1 Find the critical height r_C up the tower, measured from Earth's center, at which the object would have to be released from rest to escape Earth's gravity. 0.5pt

Building a tower of greater height than r_G is necessary if we wish to use it to launch spacecraft on voyages to other planets. Given that the tower height is 107000 km from Earth's center.

4.2 Find the minimal and the maximal distances from the Sun that a spacecraft released from rest from the top of the tower can reach. Give your answers in astronomical units. We neglect the Earth's gravitational attraction at this height. 1.0pt

Thermoelectric effects and their applications in thermoelectric generator and refrigerator (10 pt)

Introduction: Thermoelectric effects

Thermoelectric effects in conducting materials are due to the interplay between heat current and electrical current. In this problem we consider only three predominant thermoelectric effects, namely the Joule, the Seebeck and the Peltier effects, neglecting the others.

The Joule effect is a consequence of the interaction between electrical carriers and crystal lattice. Moving directionally in presence of electrical current, carriers transfer a part of their energy to the vibrating crystal lattice, and as a result the crystal is heated. The Joule effect is irreversible.

The Seebeck effect can be observed in a thermocouple consisting of two dissimilar conducting bars A and B connecting by direct junction (Fig. 1a) or junction via an intermediate material C (Fig. 1b). The material C is good electrical conductor with very small specific heat. When the two junctions of the thermocouple are maintained at different temperatures T_{1} and T_{2} (Fig. 1a,b) the Seebeck electromotive force (*emf*) is produced

$$
\epsilon = \alpha (T_1 - T_2) \tag{1}
$$

where α is the Seebeck coefficient of the thermocouple. α is considered temperature independent.

The Seebeck effect is applied in thermoelectric generator to convert heat energy into electrical one.

Figure 1. (a) direct junctions. (b) junctions via an intermediate material C. (1) Heat source (temperature T_1); (2) Heat sink (temperature $T_2^{}$)

The Peltier effect

Whenever current passes through a thermocouple circuit consisted of two dissimilar conductors A and B with direct junctions (Fig. 2a) or junctioned via intermediate conductor C (Fig. 2b), depending on the

current direction, heat is either absorbed or released at the junctions of the two conductors. This is the Peltier effect. The Peltier heat power *q* appeared at a junction is

$$
q = \pi I \tag{2}
$$

 π is the Peltier coefficient of this junction.The Seebeck and Peltier effects are reversible effects in contrast to the irreversible Joule effect. Although the Seebeck and Peltier effects need junctions between the thermoelements, they are essentially bulk effects. A closed electrical cycle in a thermocouple with the Peltier effect (Fig. 2b) can be used as a refrigerator when heat is removed from one isolated junction and rejected at the other.

For simplicity, the heat radiation, circulation, conduction through surrounding environment are considered negligible, and heat current is supposed to be inside the thermocouple and at the heat source and the heat sink.

Figure 2. (a) Direct junctions; (b) junctions via an intermediate material C

Data for thermal and electrical properties of materials and the thermocouple studied in this problem are given in the Table 1 and 2 for numerical calculation.

Name	Material		$^{\prime}$ Resistivity ρ ($\Omega \cdot \mathrm{m})\,$ Thermal conductivity k ($\mathrm{W} \cdot \mathrm{m}^{-1} \cdot \mathrm{K}^{-1})\,$ \vert
	$\text{Bi}_2\text{Te}_{2.7}\text{Se}_{0.3}$	1.0×10^{-5}	
	$\text{Bi}_{0.5}\text{Sb}_{1.5}\text{Te}_{3}$	1.0×10^{-5}	I .4

Table 1: Parameters of materials used in thermocouple (at room temperature)

Table 2: Parameters of the thermocouple.

A. Heat transfer and thermoelectric generator

A1. Heat transfer in a homogeneous conducting bar

An electric current I (Figure 3) flows along a homogeneous conducting bar with length L, resistivity ρ , thermal conductivity *k*. The two ends of the bar are located at coordinates $x = 0$ and $x = L$ in the OX axis. The temperature at $x=0$ is T_1 , at $x=L$ is $\,T_2\,(T_1>T_2)\,$, both temperatures are kept constant.

Figure 3

The heat current $q(x)$ (the amount of heat transferred via perpendicular cross-section per unit time) flowing in the bar is described by the Fourier law

$$
q(x) = -kS \frac{dT(x)}{dx}
$$
 (3)

here k is thermal conductivity, and S is the cross-sectional area of the bar.

- **A1.1** Find the temperature distribution $T(x)$ when x varies along the bar at the steady state assuming no heat loss to the surroundings. *Hint: the equation* $\frac{d^2T(x)}{dx^2} = a$ *has the solution* $T(x) = \frac{1}{2}ax^2 + C_1x + C_2$ *, where* C_1 and C_2 are derived from boundary conditions. 0.75pt
- **A1.2** Find the heat current $q(x)$ at point x and $q(0), q(L)$ at the two ends, respectively. 1.0pt

A2. Relation between Peltier and Seebeck Coefficients

Relation between Peltier and Seebeck coefficients for all temperature range is generally proved in thermodynamics. Here, this relation is derived for the particular case when the thermocouple is made of conducting materials A and B (Fig.1b) with the Seebeck coefficient α and small-enough resistivity so that the Joule effect can be neglected. The Peltier coefficients at the hot (temperature T_1) and cold (temperarure T_2) junctions are π_1 and π_2 correspondingly. During electrical process, the electron gas in the thermocouple performs a ideal thermodynamic cycle.

A2.1 Find the expression for the heat current received by the electron gas from the heat source with temperature $T_1.$ 0.25pt

- **A2.2** Find the expression for the heat current transferred by the electron gas to the heat sink with temperature $T_2.$ 0.25pt
- **A2.3** Find the net electrical power produced by the electron gas if the Seebeck coefficient is α . 0.5pt
- **A2.4** Express the Peltier coefficient π at a junction in term of the Seebeck coefficient α and the temperature T of the junction. 0.5pt

A3. Thermoelectric generator

Figure 4. Thermoelectric generator. (1) Heat source (temperature T_1); (2) Heat sink (temperature T_2).

Hereafter the Peltier coefficient π is taken to be equal to αT for all temperatures and the Joule heat must be *included in consideration.*

The thermocouple consistsing of two conducting bar A and B with equal lenght L is used as thermoelectric generator (Fig. 4). The parameters of the bars A and B are: cross-sectional areas S_A , S_B ; resistivities $\rho_A, \, \rho_B$; thermal conductivities $k_A, \, k_B.$ The lower ends of the A and B bars are connected to a load of resistance $R_L.$ Parameters of the thermocouple are: α the Seebeck coefficient, $R=\frac{\rho_A L}{S_A}+\frac{\rho_B L}{S_B}$ the internal resistance, $K=\frac{k_A S_A}{L}+\frac{k_B S_B}{L}$ the thermal conductance. The upper hot end (lower cold end) of the thermocouple is maintained at temperature $T_1(T_2)$ and $T_1>T_2.$ Denote q_1 as the heat power taken from the heat source with temperature $T_1,\,q_2$ as the heat power transferred to the heat sink with temperature T_2 by the themocouple.

A3.1 Find the expressions for q_1,q_2 in terms of the thermocouple parameters $\alpha, K, R,$ the temperatures $T_1,\,T_2$ and the current I 0.5pt

The efficiency of the thermoelectric generator is defined as η $=$ $\frac{P_L}{q_1}$, where P_L the electrical power of the load. The ratio between the load and internal resistances of the thermocouple is denoted as $m\!=\!\frac{R_L}{R}$

A3.2 Find the expression for the efficiency η in terms of the thermocouple parameters $\alpha, K, R,$ the temperatures $T_1,$ T_2 and the resistance ratio m 0.75pt

In order to determine the efficiency of thermoelectric generators, the following properties of the thermocouple are needed: low electrical resistance to minimize Joule heating, low thermal conductivity to retain heat at the junctions, and a maintained large temperature gradient. These three properties are put together in one quantity $Z=\frac{\alpha^2}{KR}$, which is called the figure-of-merit of the thermocouple.

A3.3 Find the expression for the efficiency in terms of Z , the ideal Carnot cycle efficiency $\eta_c = \frac{T_1 - T_2}{T_1}$, T_1 and m . 0.25pt

A4. The maximum efficiency

The efficiency of the thermocouple equals η_P when the electric power of the load takes the maximum value, $P_L = P_{\text{max}}$.

The efficiency is maximum $\eta = \eta_{\sf max}$ when the resistance ratio *m* takes some value which is denoted by M.

A4.3 Express the maximum efficiency $\eta_{\sf max}$ via T_1, T_2, Z and M . $\hspace{1.6cm}$ 0.25pt

A5. **The maximum figure of merit**

Increasing the figure of merit of the thermocouple leads to the increase of the efficiency of the thermoelectric generator. In practice, the cross-sectional areas S_A , S_B of the bars of the thermocouple are choosen so that the figure of merit of the thermocouple has maximum value $Z = Z_m$

- **A5.1** Derive the expression for the ratio between the cross-sectional areas $\frac{S_A}{S_B}$ of the bars in terms of ρ_A , ρ_B , k_A , k_B when the figure of merit of the thermocouple is maximum. 0.5pt
- **A5.2** Express the maximum figure of merit Z_m in term of $\alpha, \rho_A, \rho_B, k_A, k_B$ (0.25pt

A6. **The optimum efficiency**

The optimum efficiency η_{opt} of the thermolectric generator is defined as the efficiency when the electric power at the load and the figure of merit both are at the maximum values. The hot heat source and cold heat sink are maintained at temperatures $T_1 = 423 \text{ K}, T_2 = 303 \text{ K}$ respectively.

- **A6.1** Find the numerical value η_{opt} of the thermoelectric generator made from materials with parameters given in Table 1 and compare it with the ideal efficiency η_c . 0.5pt
- **A6.2** Find the numerical value of the maximum efficiency η_{max} of the thermoelectric generator made from given materials. 0.25pt

B. Thermoelectric refrigerator

The thermocouple with parameters α , K, R given in the question A3 is used as a thermoelectric refrigerator and described in the Fig.5.

B1. The cooling power and the maximum temperature difference

The upper end of the thermocouple is a heat source with the initial temperature T_1 . It is thermally isolated with ambient environment, and needs to be cooled. The lower ends of the thermocouple, A and B bars are connected to a battery and are at the temperature $T₂$ of the heat sink. The sense of the electrical current is chosen so that the Peltier heat is absorbed at the upper junction and released to the heat sink at the lower junction.

Figure 5. Thermoelectric refrigerator. (1) Isolated heat source (temperature T_1); (2) Heat sink (temperature $T_2^{}$)

B1.1 Find the expression for the cooling power q_C (heat current flows from the heat source to the bars of the thermocouples) in terms of the thermocouple parameters α, K, R and T_1, T_2, I . 0.25pt

B1.2 Find the expression for the maximum temperature difference $\Delta T_{\text{max}} = T_2 - T_1$ $T_{1 \text{min}}$ in term of the figure of merit *Z* of the thermocouple and the lowest temperature of the isolated heat source $T_{1\text{min}}$. 0.5pt

B2. The working current

The thermocouple made from materials A and B with best value of figure of merit Z_m found in part A is used for the refrigerator.

- **B2.1** Calculate the numerical value of the minimum temperature of the isolated heat source $T_{1\text{min}}$ if the temperature of the heat sink is $T_2 = 300K$. 0.25pt
- **B2.2** Calculate the working current intensity I_w of the thermoelectric refrigerator when the temperature of the heat source is at the minimum value $T_{1\text{min}}$ and the temperature of the heat sink $T_2 = 300K$. For simplicity the cross-sectional areas of the bars are taken to be equal, $S_A=S_B=10^{-4}m^2\overline{2}$ 0.5pt

B3. The coefficient of performance

When the temperature difference is less than its maximum value ΔT_{max} , the coefficient of performance β is usually used for assessing of the performance of the thermoelectric refrigerator. β $=$ $\frac{qc}{P}$, where P is the supplied electrical power.

B3.1 Find the expression for the coefficient of performance β in terms of the parameters $\alpha, \, K, \, R$ of the thermocouple and $T_1, \, T_2, \, I.$ 0.5pt

When the coefficient of performance has its maximum value β_max , the current intensity is I_β .

B3.2 Find the expression for I_β in terms of the parameters $\alpha,$ $Z,$ R of the thermocouple and temperatures $T_1,\,T_2.$ 0.25pt

B3.3 Find the expression for the maximum coefficient of performance β_{max} . 0.25pt